Turbulent Flame Speeds and NOx Kinetics of HHC Fuels with Contaminants and High Dilution Levels

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TEXAS A&M UNIVERSITY

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Project Overview

First Year of Three-Year Project is Complete

Project Highlights:

1. Duration: **Oct. 1, 2010 – Sept. 30, 2013**

2. DOE NETL Award **DE-FE0004679**

3. Budget: $501,712 DOE + $125,500 Cost Share

4. Principal Investigator: Dr. Eric L. Petersen

5. Participating Organizations:
   - Rolls-Royce (Dr. Gilles Bourque)
   - The Aerospace Corporation (Dr. Mark Crofton)
   - Trinity College (Dr. John Mertens)

Project Overview

This Project Addresses Several Problems for HHC Fuels

1. Improve **NOx kinetics** for High-Hydrogen Fuels at Engine Conditions

2. Effect of **Contaminant Species** on Ignition

3. Impact of **Diluents** on Ignition Kinetics and Flame Speeds

4. Data on **Turbulent Flame Speeds** at Engine Pressures

Project Overview

There are Six Main Work Tasks for the Project

Work Tasks:

Task 1 – Project Management and Program Planning

Task 2 – Turbulent Flame Speed Measurements

Task 3 – Laminar Flame Speeds with Diluents

Task 4 – NOx Mechanism Validation Experiments

Task 5 – Fundamental NOx Kinetics

Task 6 – Effect of Impurities on Syngas Kinetics

Task 1 – Project Management and Program Planning

Project Participants

Dr. Olivier Mathieu

Michael Krejci

Christopher Aul

Sankar Ravi

Anthony Levacque

Andrew Vissotski

John Pemelton

Travis Sikes

Aerospace Corp: Mark Crofton, Andrea Hsu

Task 1 - Management

Interaction and Feedback from Industry Will be Important

Industrial Advisory Panel

Rolls-Royce Canada:
Dr. Gilles Bourque

Siemens:
Dr. Scott Martin
Dr. Ray Laster

General Electric:
Dr. Hasan Karim
Mr. Joel Hall

Power Systems Mfg.:
Dr. Peter Stuttaford
Mr. Khalid Oumejjoud

- Mixture Compositions and Test Conditions

- Possible Contaminant Species

- Important, Related Aspects and Ultimate Usage of Models

Task 2 – Turbulent Flame Speed Measurements

Task 2 – Turbulent Speeds

Turbulent Flame Speed Measurement will Require Development of Techniques

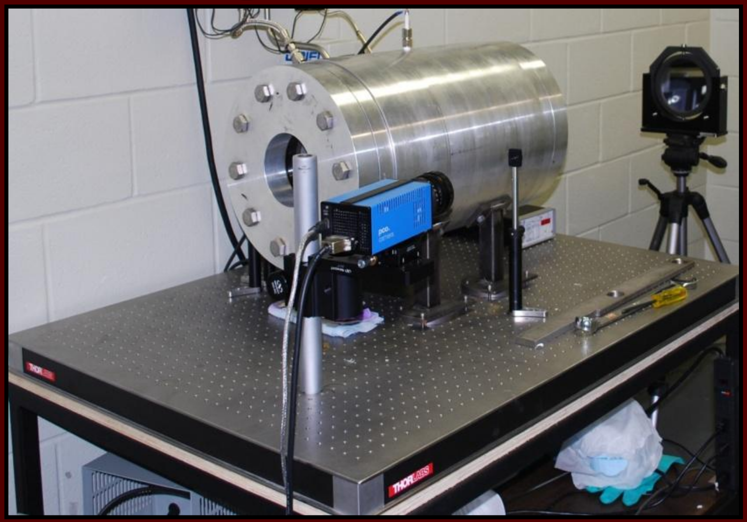
- Utilize Existing Flame Speed Hardware
- Induce Turbulence Using Fans
- Similar to Bomb Experiments of Kido and Coworkers
- Coordinate with Ongoing UTSR Projects Using Other Methods

Goal: Independent Control of Length Scale and Frequency

Task 2 – Turbulent Speeds

Design Modifications for Turbulence Production are being Optimized Using a Mock-Up Rig

Rig to be Modified



Mock-Up Rig

1. Optically Accessible for PIV
2. Similar Geometry as AL Rig
3. Frees up Rig While Turbulence Generation is Optimized

Task 2 – Turbulent Speeds

Design of Experiments Approach is Used to Explore the Range of Fan Details

Factors Varied

1. Fan OD (Inches)
2. Number of Blades
3. Blade Pitch (Degrees)

Factors Held Constant

1. Fan Placement (Central)
2. Number of Fans (4)
3. Fan Axial Length (1.5 in)

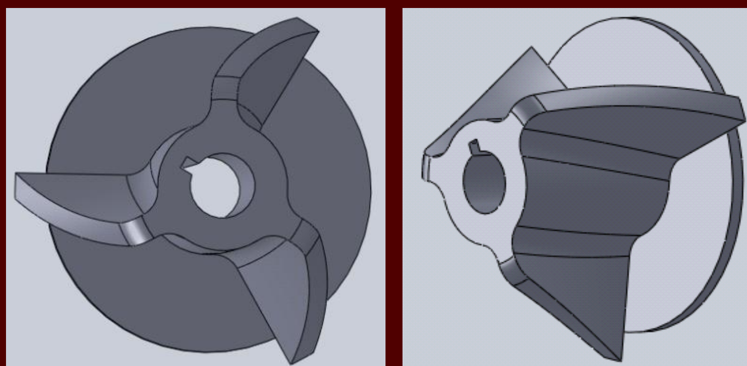
Design of Experiments Matrix (L4):

Prototype	Fan OD	No of Blades	Blade Pitch
1	3	3	20
2	5	3	20
3	3	6	20
4	3	3	60

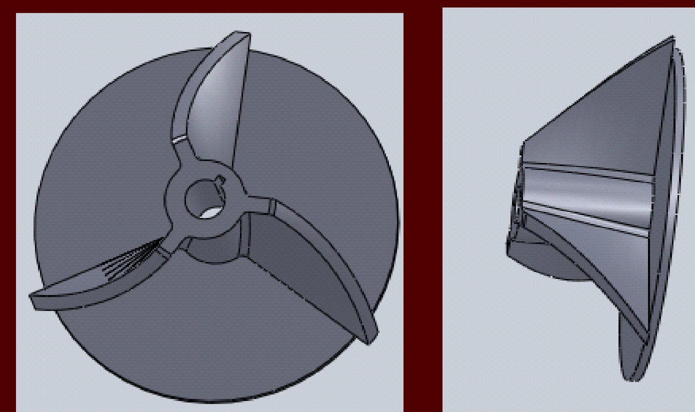
Task 2 – Turbulent Speeds

Fan Blade Designs Manufactured Using Rapid Prototyping

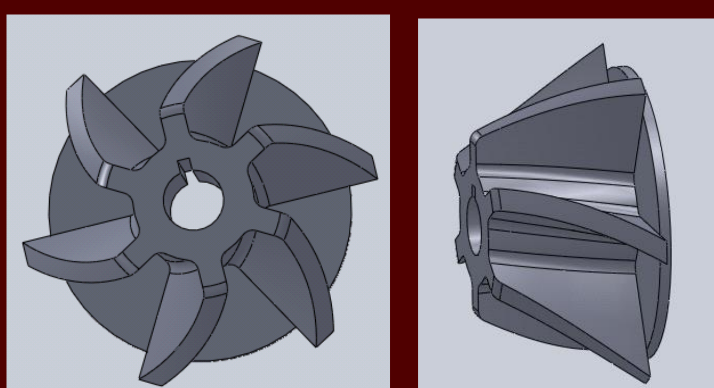
PROTOTYPE 1



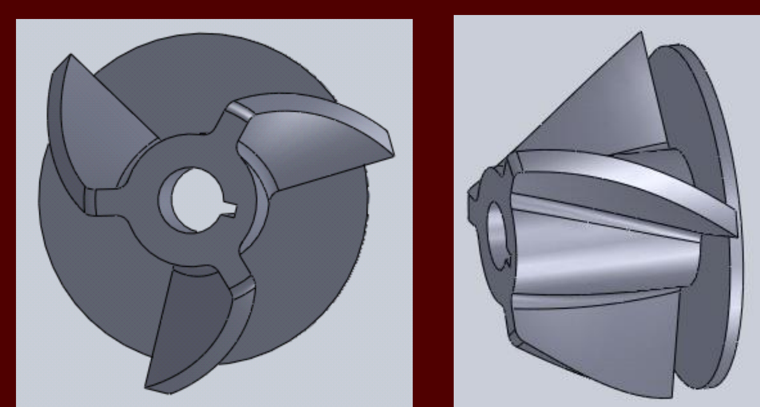
PROTOTYPE 2



PROTOTYPE 3



PROTOTYPE 4



Task 2 – Turbulent Speeds

Year 2 *Will Include a Finished Design and Shakedown of New Turbulent Flame Speed Capability*

- Complete Design Optimization Experiments
- Design and Assemble New Fans for High-Pressure Rig
- Characterize Turbulence Generation of New Facility
- Perform Shakedown Experiments Using H_2-Air Mixtures

Task 3 – Laminar Flame Speeds with Diluents

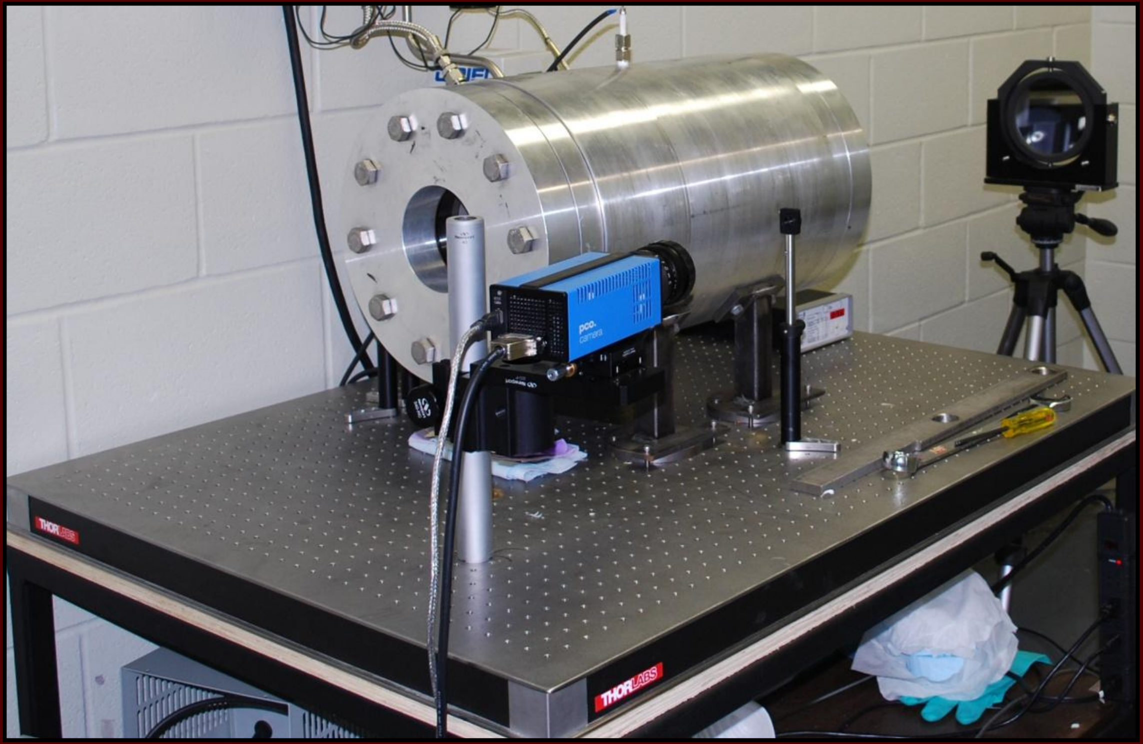
Task 3 – S_L with Diluents

High-H_2 Fuels with High Levels of Dilution Will be Studied

- Water, CO_2, N_2, other?
- Laminar Flame Speeds Using Established Methods
- Utilize New Heated Vessel for Water Mixtures
- Pertinent Mixtures of Interest to Industry

Task 3 – S_L with Diluents

Original Vessel Capable of High-Pressure Tests but is Not Heated



- Vessel ID 31.74 cm
- Internal Length 35.6 cm
- 6 cm Thick Fused Quartz Windows
- 12.7 cm Diameter Windows
- Max Test Pressure ~ 20 atm
- Minimum Safety Factor of 4

Task 3 – S_L with Diluents

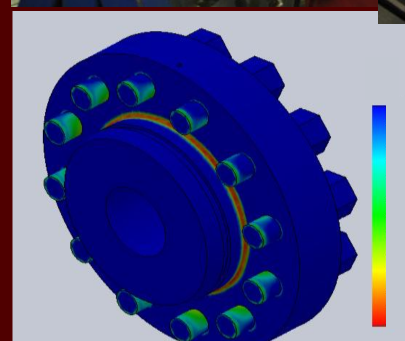
New High-Temperature High-Pressure Flame Speed Vessel is Now Operational

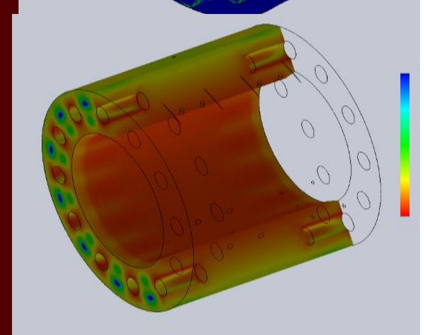
Design Parameters:

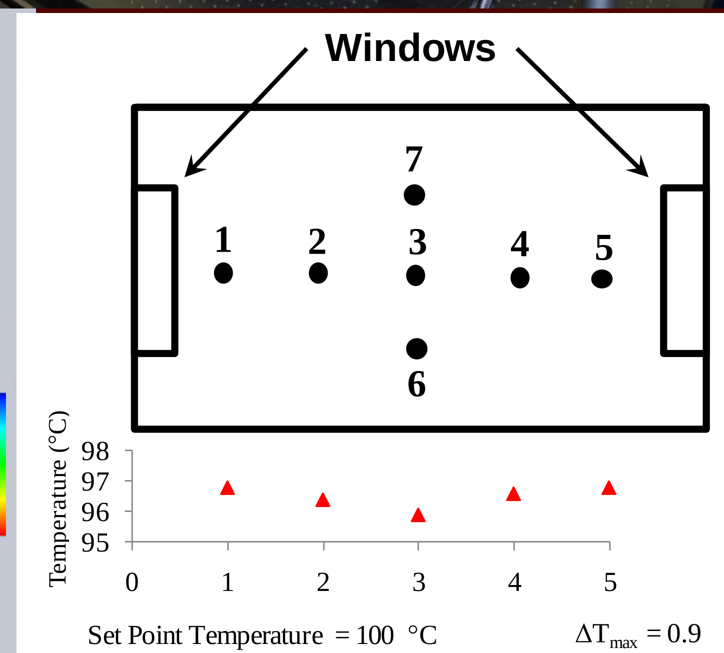
- *Max initial pressure:* ***30 atm***
- *Max initial temperature:* ***600 K***

Vessel Dimensions:

- *Outer Dia.: 54.6 cm*
- *Inner Dia.:* ***31.8 cm***
- *External Length: 63.5 cm*
- *Internal Length:* ***27.9 cm***
- *Window Port Dia.: 12.7 cm*
- *Approximate Wt: 1800 lbs*



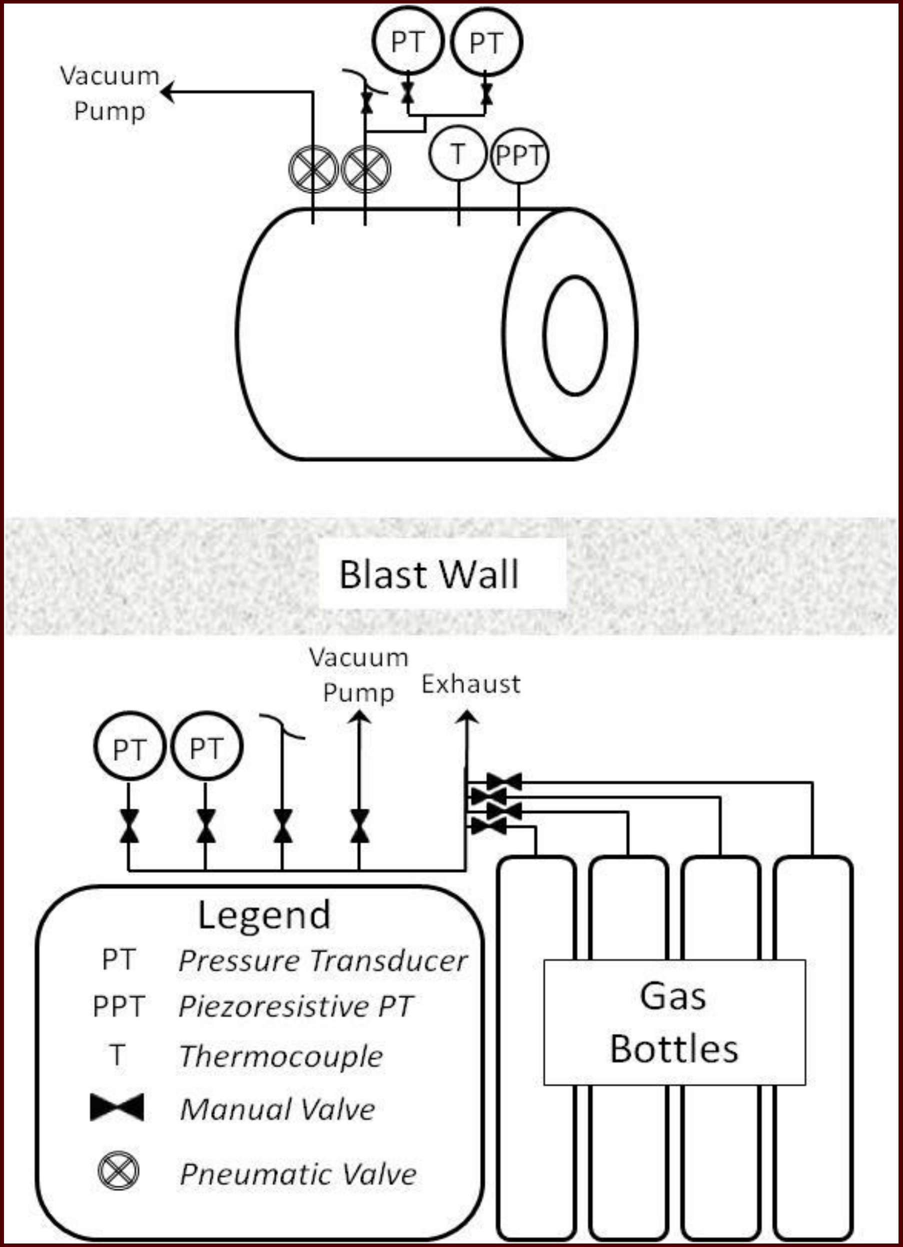




Task 3 – S_L with Diluents

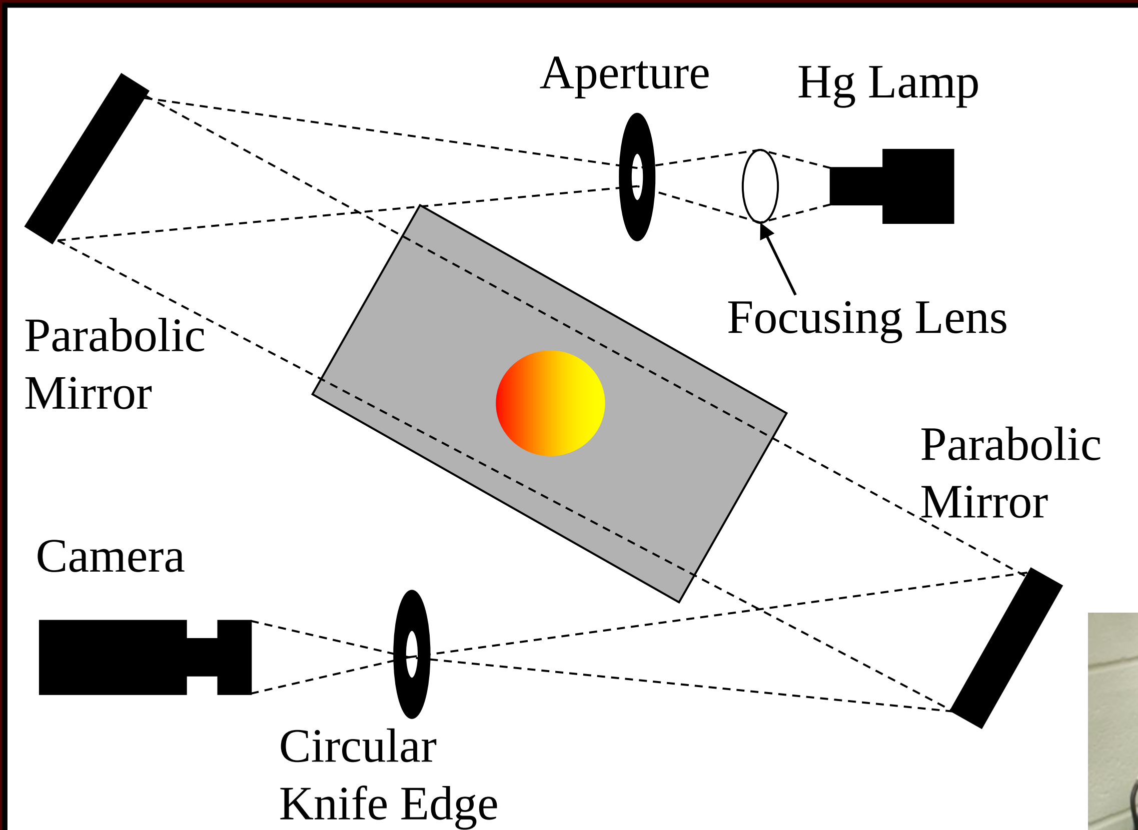
HTHP Facility Infrastructure

- 5 Pressure Transducers (PT)
- 1 Thermocouple (T)
- 2 Vacuum Pumps
- 4-Piece Heating Jacket
  - Temperature Controller adjusts by 1° Increments

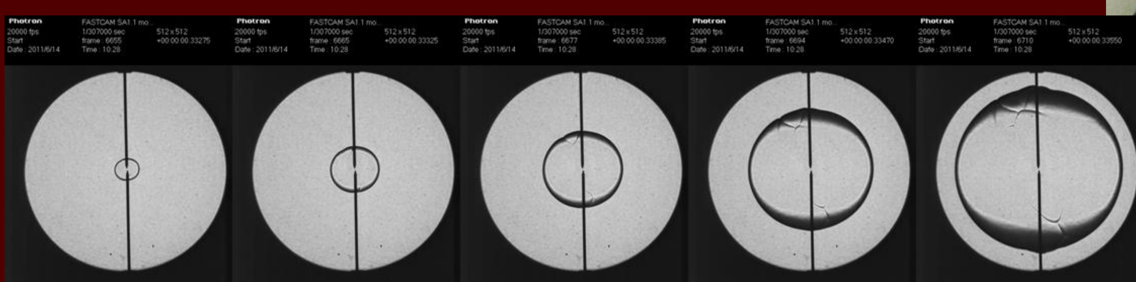


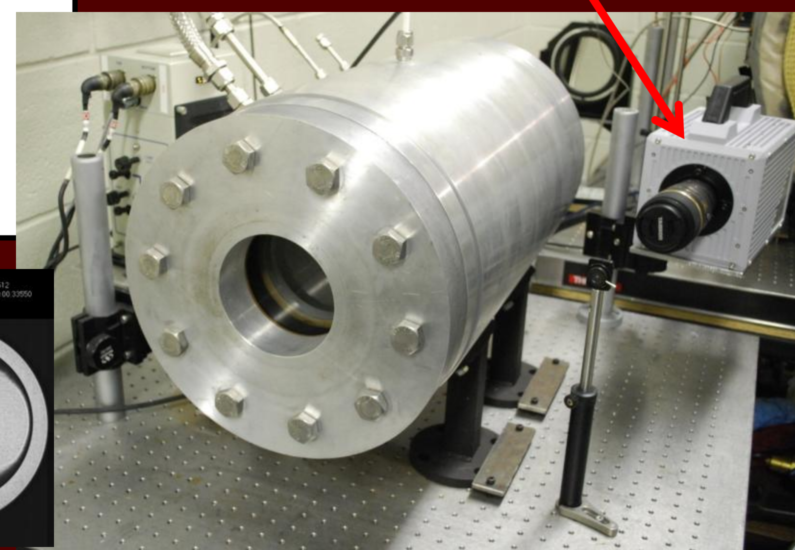
Task 3 – S_L with Diluents

Z-Type Schlieren Setup Used to Obtain Flame Growth



- f/8 Mirrors. (Dia. 6 in)
- Mercury Lamp
- New Photron Fastcam SA1.1





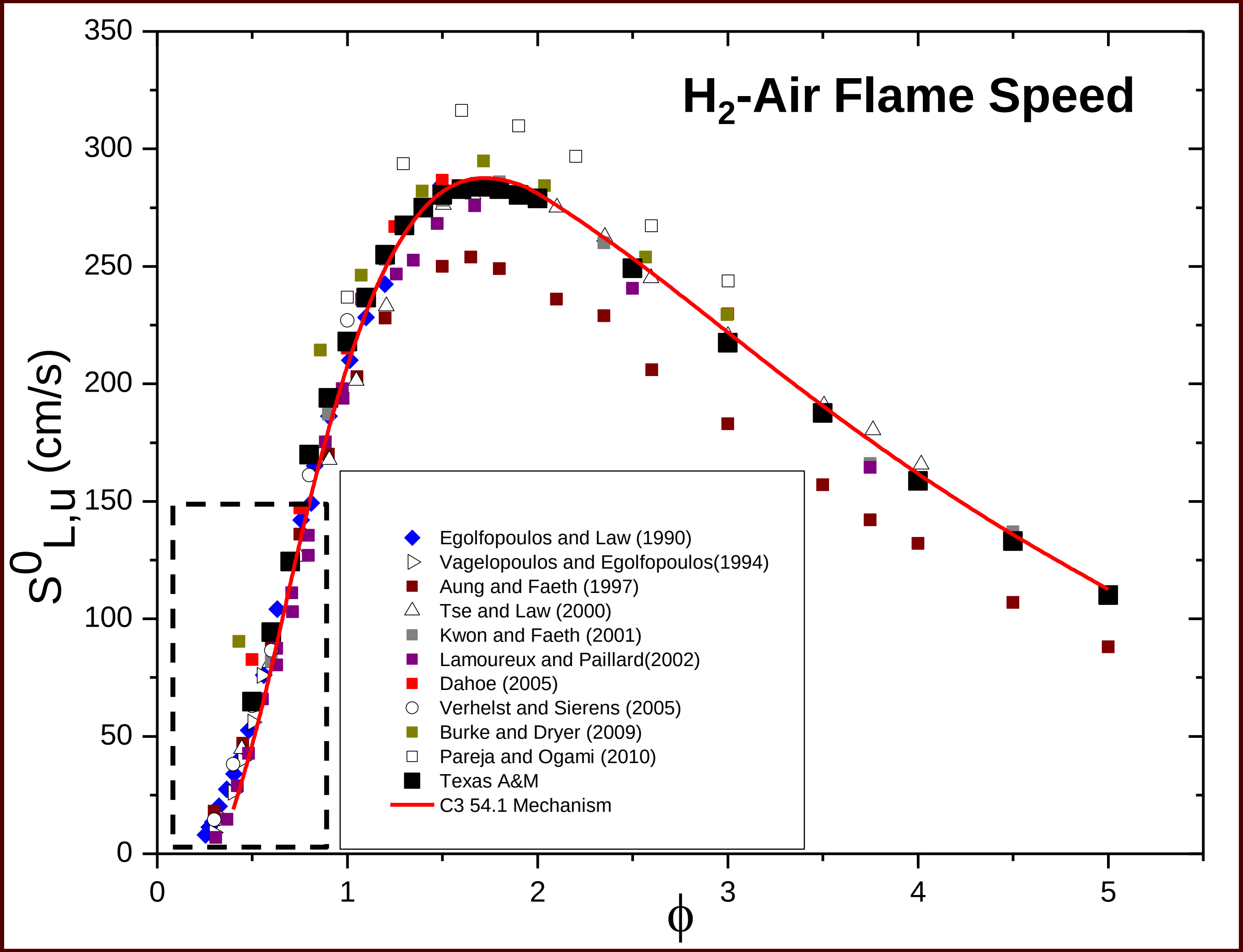
Task 3 – S_L with Diluents

***Test Plan** Includes a Series of **Baseline** Experiments with H_2 and H_2-CO Mixtures in Air*

- Pure H_2 in Air Experiments to Compare with Literature
- Core Chemical Kinetics Model Based on Work with NUI Galway
- 50:50 CO-H_2 Mixtures Tested
- Diluent Study with H_2O, CO_2 to be Based on Statistical Matrix

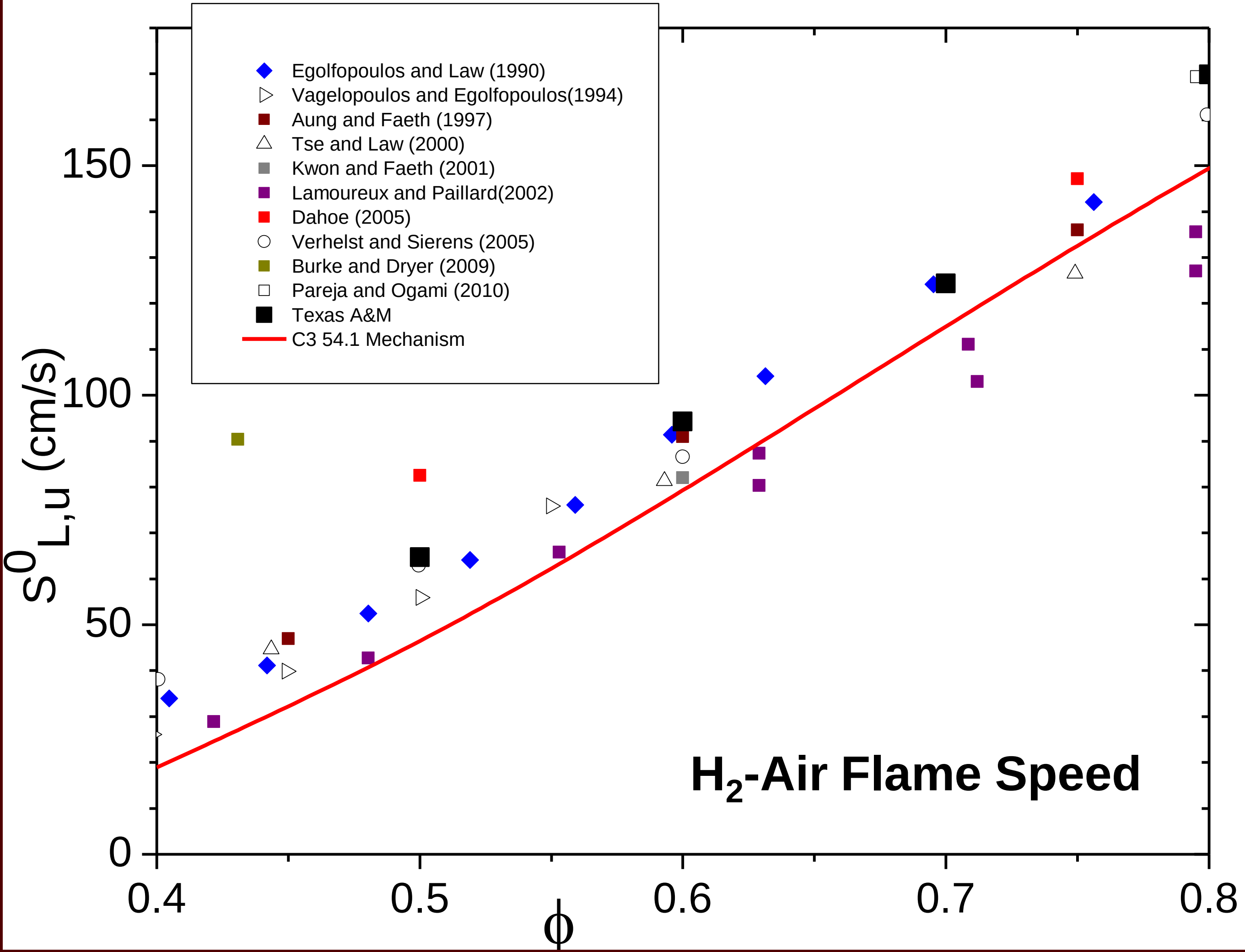
Task 3 – S_L with Diluents

1-atm H_2 Results *Compare Well with Model and Literature*



Task 3 – S_L with Diluents

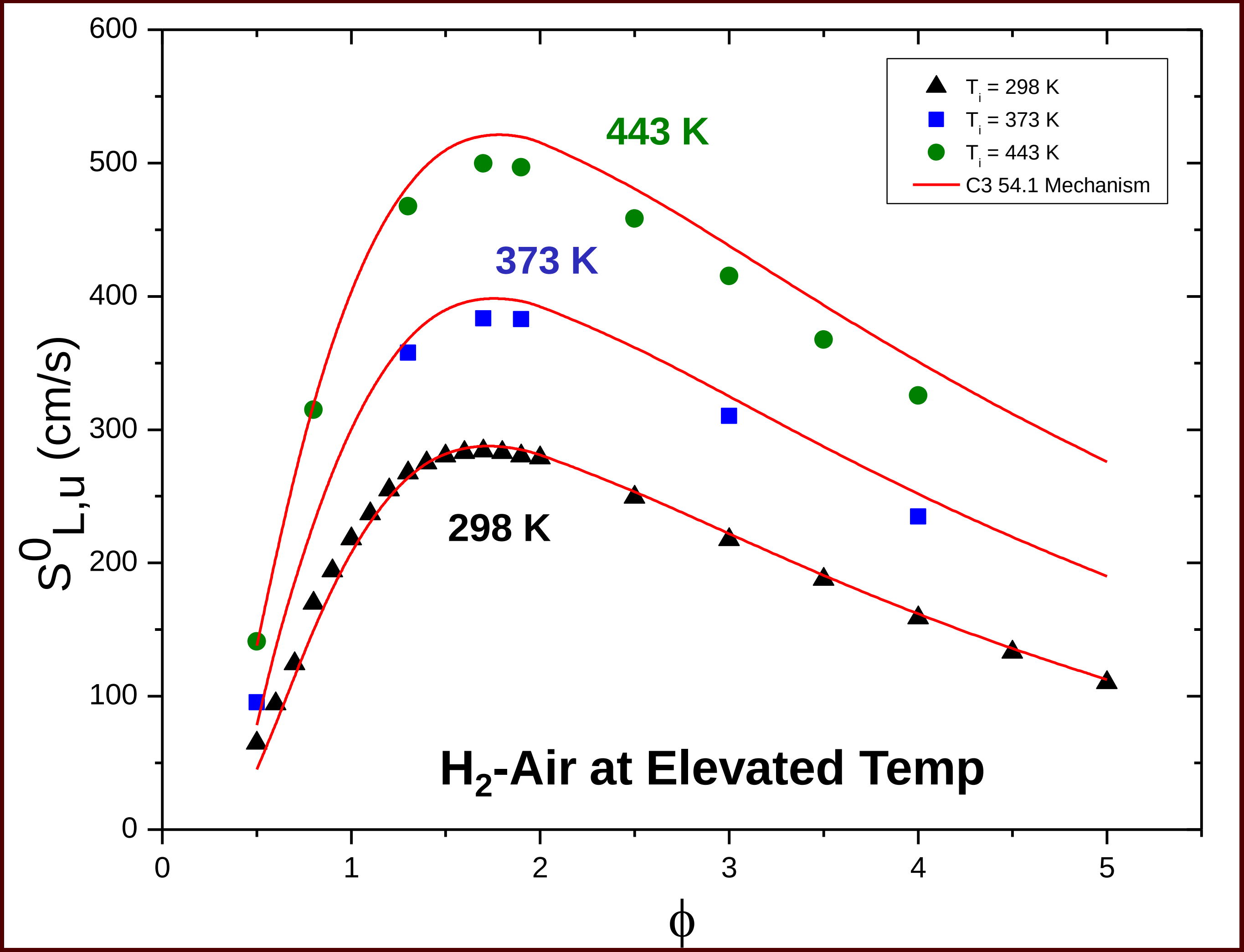
Closer Look Shows 20+ cm/s Scatter at Lean Conditions



- Model Underpredicts by 10-20 cm/s
- 30-cm/s Variation Amongst data
- How Accurate do we Need to be?

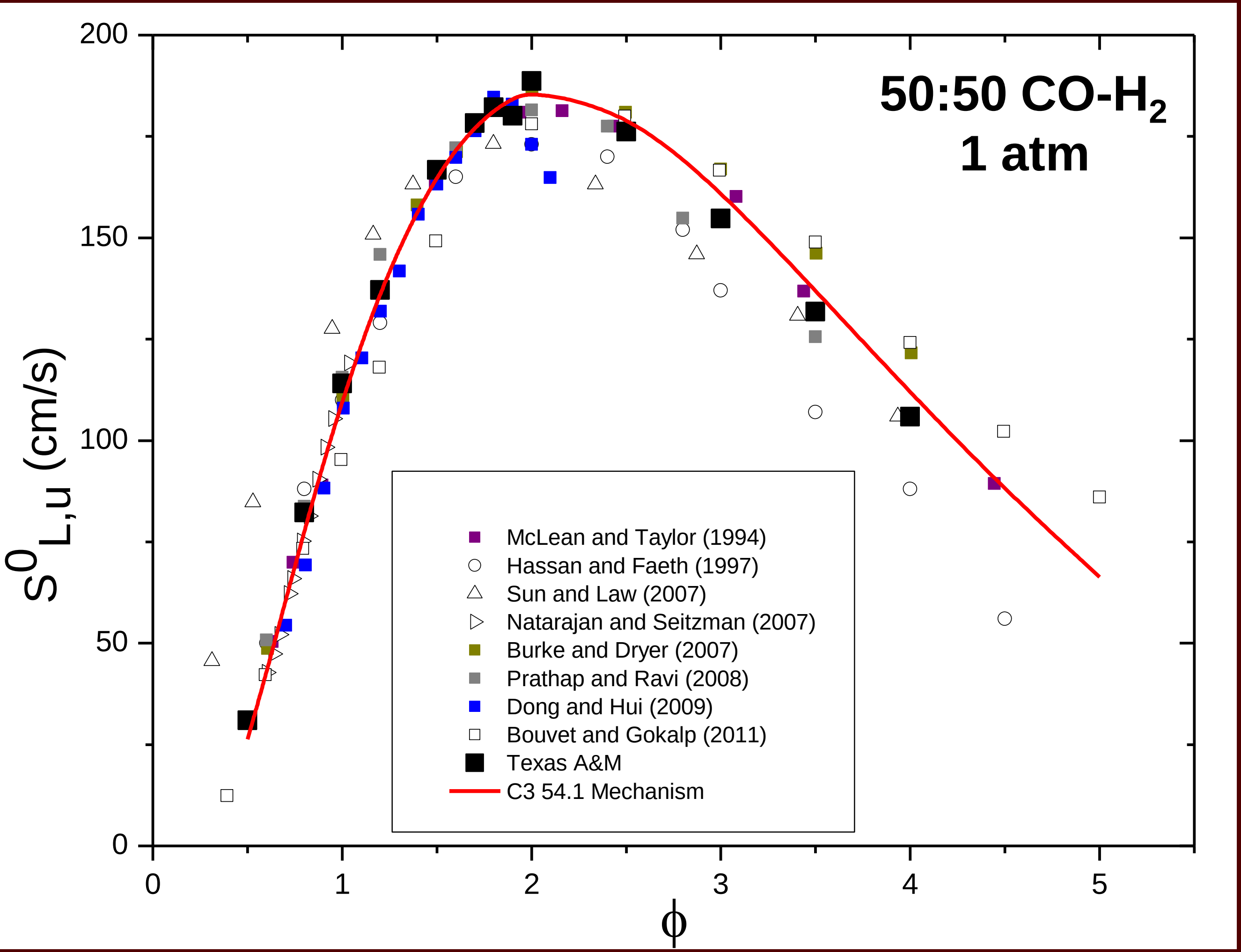
Task 3 – S_L with Diluents

Elevated-Temp. H_2 Results *Compare Well with Model*



Task 3 – S_L with Diluents

CO-H_2 Results *Have Several Studies for Comparison*



Task 3 – S_L with Diluents

Ongoing Experiments to Include H_2O Using a Design of Experiments Approach

Experiment	Temperature (K)	Pressure (atm)	%H2O (by mol)	H2:CO
1	323	1	7.5	5:95
2	323	5	0	50:50
*3	323	1	15	100:0
4	373	1	0	100:0
5	373	5	15	5:95
6	373	10	7.5	50:50
7	423	1	15	50:50
8	423	5	7.5	100:0
9	423	10	0	5:95

* Pressure was changed from 10 to 1 atm due to the high water concentration

- 4 Factors with 3 Levels Each
- L-9 Taguchi Matrix
- - Temperature (323, 373, 423 K)
  - Pressure (1, 5, 10 atm)
  - Water Content (0, 7.5, 15%)
  - H_2:CO Mixture (5:95, 50:50, 100:0)

Task 4 – NOx Mechanism Validation Experiments

Task 4 – NOx Mechanism

Kinetics Mechanism Validation with NOx at Engine Conditions is being Performed

- Mechanism Based on Galway C5 Mechanism
- Initial NOx Mechanism from Recent Dagaut and Brezinsky Work
- Ignition Times with NOx Precursors for Validation (and EGR-Related)
- Species Time Histories at Dilute Conditions
- Suggest Calibrated Mechanism at End

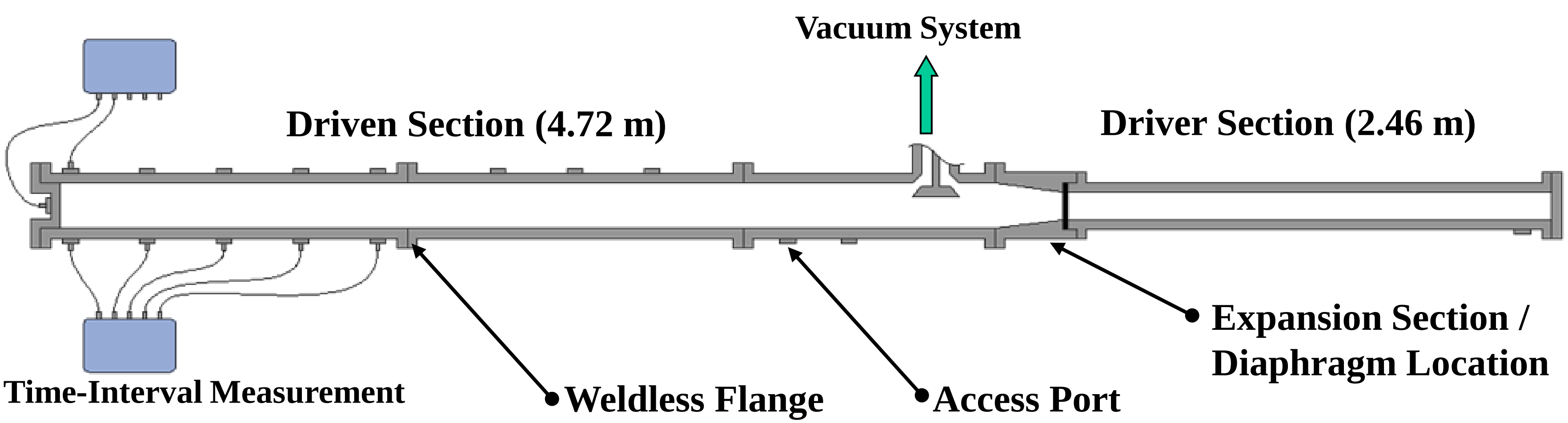
Task 4 – NOx Mechanism

Texas A&M High-Pressure Shock Tube

Task 4 – NOx Mechanism

High-Pressure Shock-Tube Facility

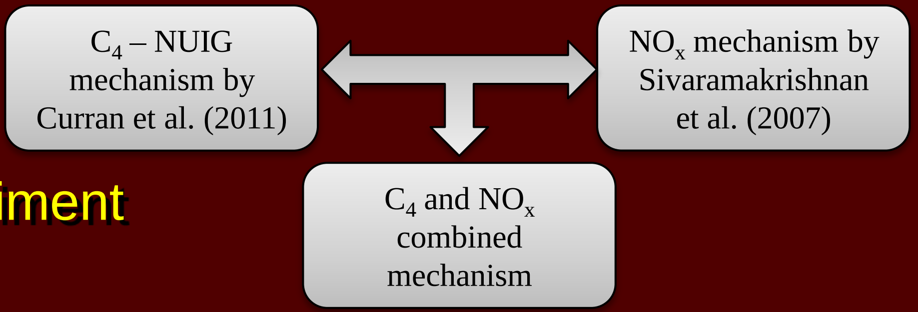
- 1 – 100 atm Capability
- 600 – 4000 K Test Temperature
- Up to 20 ms Test Time
- 2.46 m Driver and 4.72 m Driven Sections
- 15.24 cm Driven Inner Diameter



Task 4 – NOx Mechanism

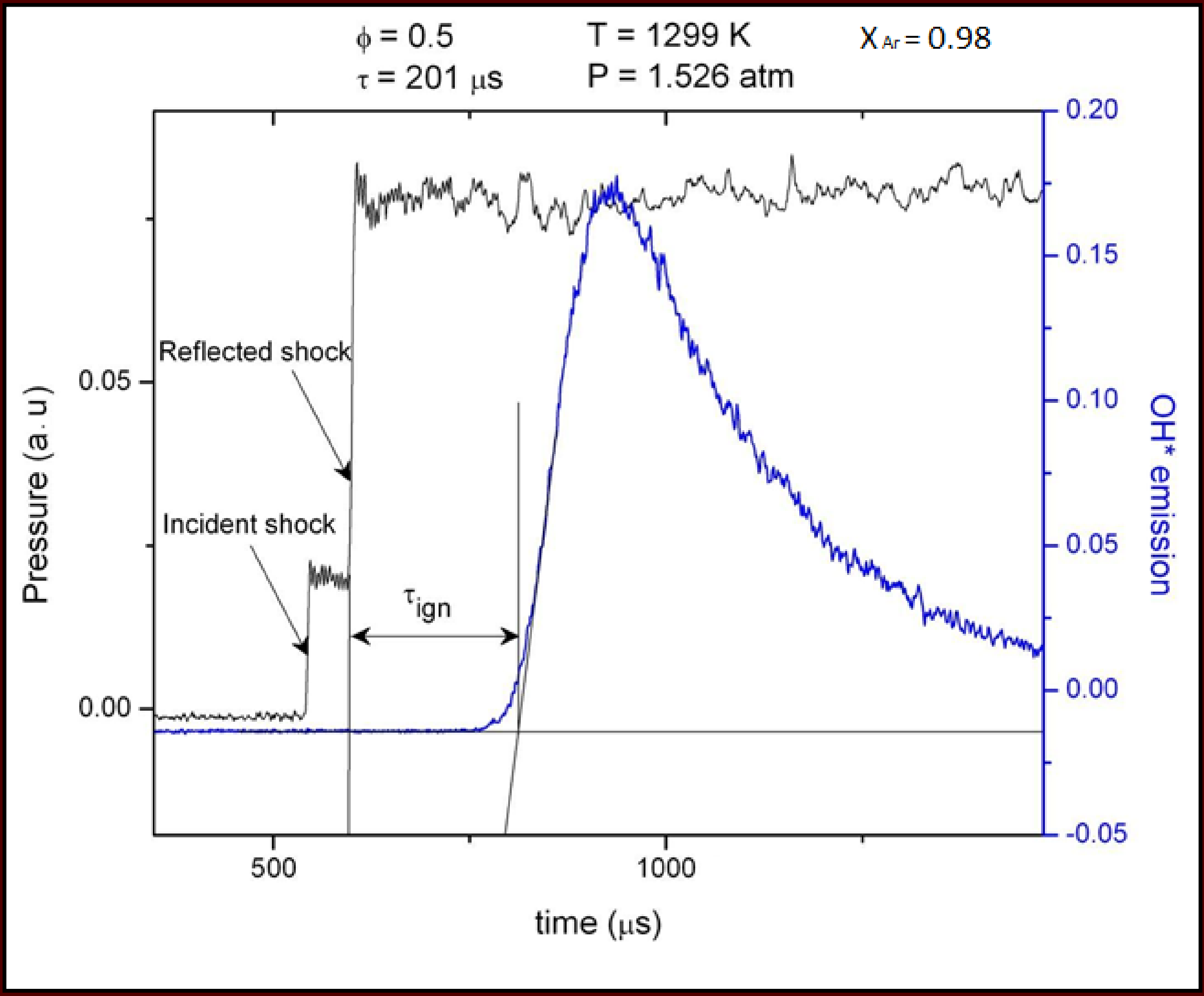
Ignition Delay Time Experiments are used to Test NOx Mechanism with H_2 Fuel

- Ignition Delay Times with and without **NO_2, N_2O**
- Baseline Fuel Mixture: **pure H_2**
- Conditions: **- 1 – 30 atm**
  - Fuel Lean
  - Dilute in Argon (98%)
- Compare Mechanism to Experiment



Task 4 – NOx Mechanism

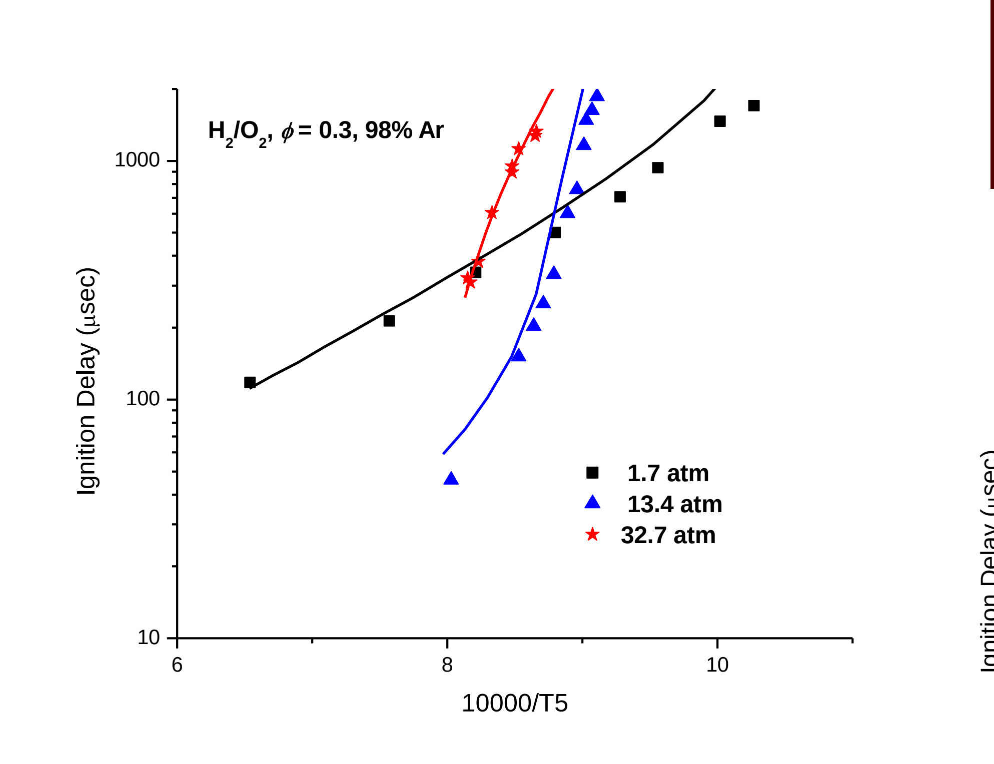
OH Used to Define Ignition in the Highly Dilute Experiments*



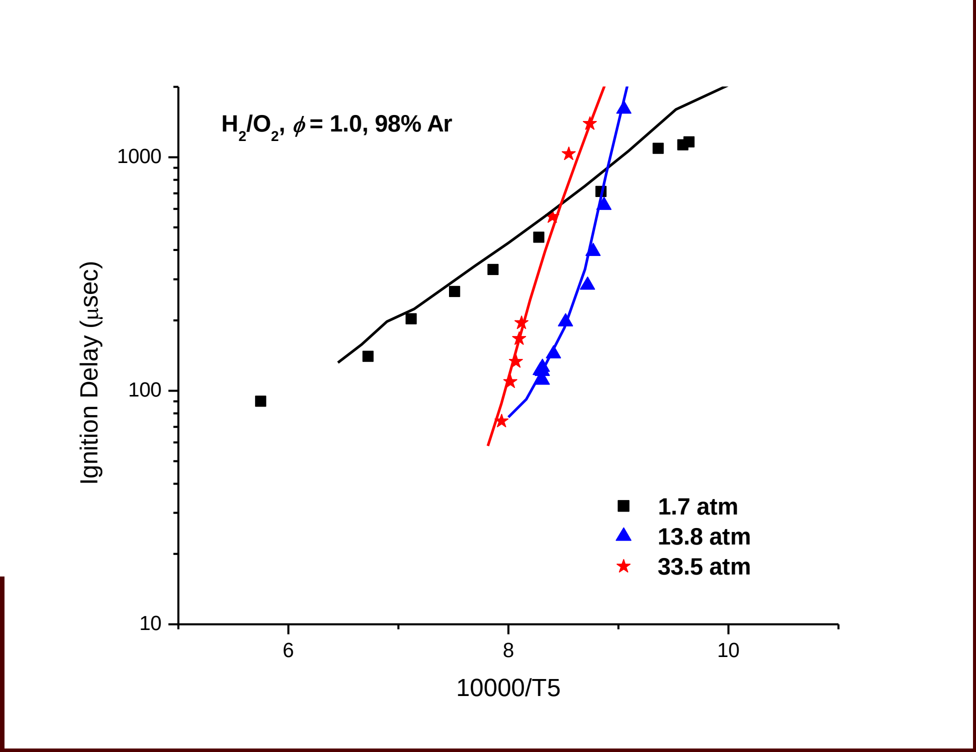
Task 4 – NOx Mechanism

Hydrogen Results Show Non-Linear Pressure Dependence

ϕ = 0.3



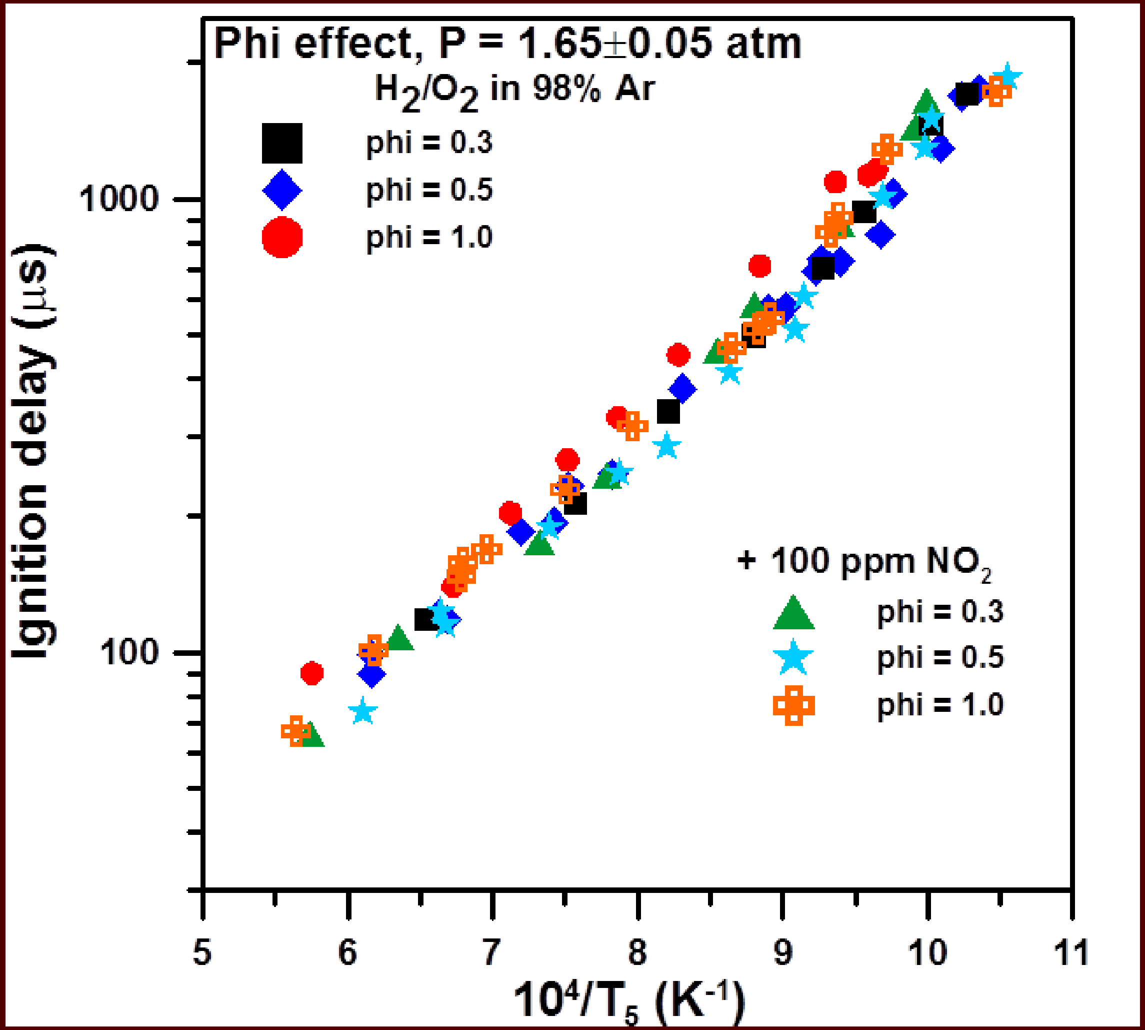
ϕ = 1.0



Task 4 – NOx Mechanism

Results Not Very Dependent on Equivalence Ratio for Hydrogen Baseline

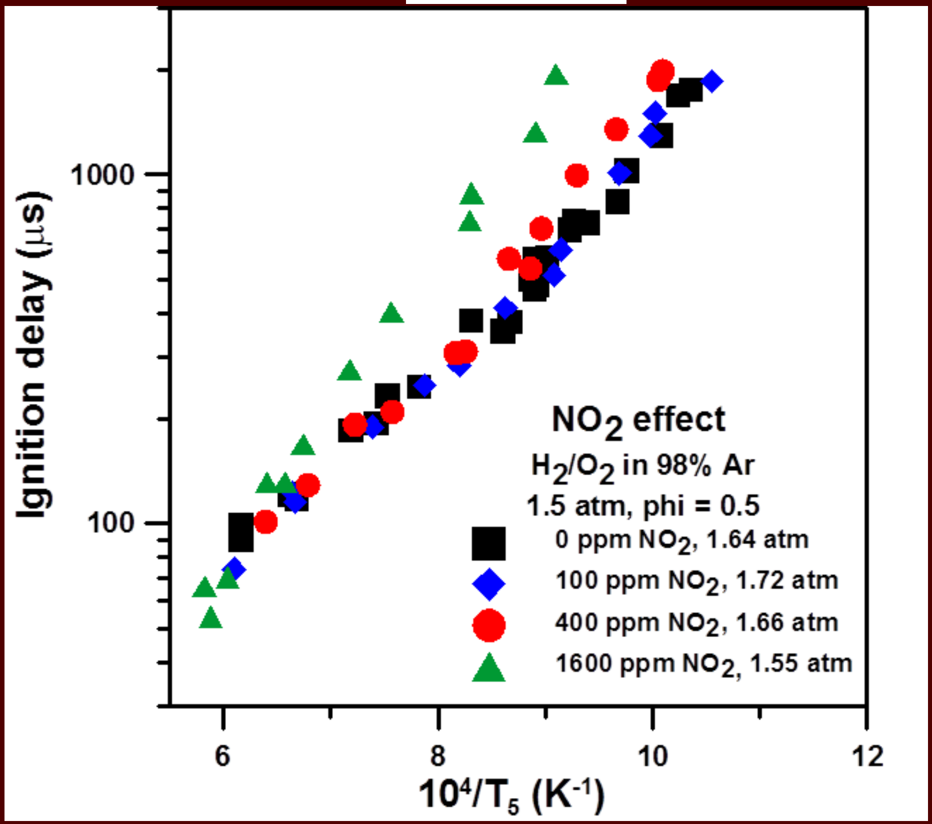
ϕ = 0.5 Chosen for Comparison with NOx Addition



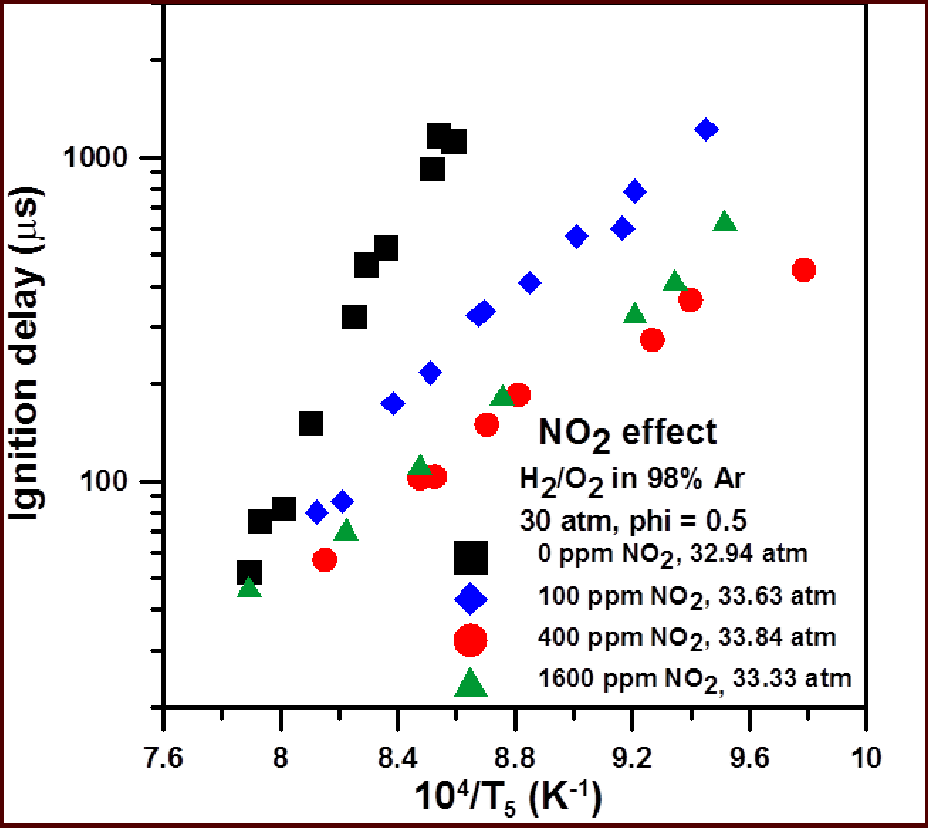
Task 4 – NOx Mechanism

Effect of NO_2 on H_2-O_2 Mixtures is Stronger at Higher Pressure

1.5 atm



30 atm



Task 4 – NOx Mechanism

Task 4 is Nearly Complete, with Current Mechanism Showing Very Good Results Overall

- Sensitivity Analysis Performed (not shown)
- Experiments Performed for N_2O Addition (not shown)
- NOx Model for Shock-Tube Conditions is in Good Shape
- NO Formation via NNH Mechanism Still Not Validated Yet (Task 5)

Task 5 – Fundamental NOx Kinetics

Task 5 – NOx Kinetics

Rate Coefficients Will be Measured Directly for Key Reactions in High-H_2 System

- Identify Specific Reaction(s) for Study
- Utilize Laser Absorption of NH (336 nm)
- Requires Very Dilute Mixtures
- Explore NNH Pathways for Prompt NOx

Task 5 – NOx Kinetics

NNH Pathway Will be the Focus of the Detailed Kinetics Experiments

- NNH Mechanism:

$$N_2 + H_2 \rightarrow NNH + H$$

$$N_2 + H + M \rightarrow NNH + M$$

$$NNH + O \rightarrow NO + NH$$

$$NNH + O_2 \rightarrow N_2O + OH$$

- Few Direct Measurements

- Study will Focus on

$$N_2 + H + M \rightarrow NNH + M$$

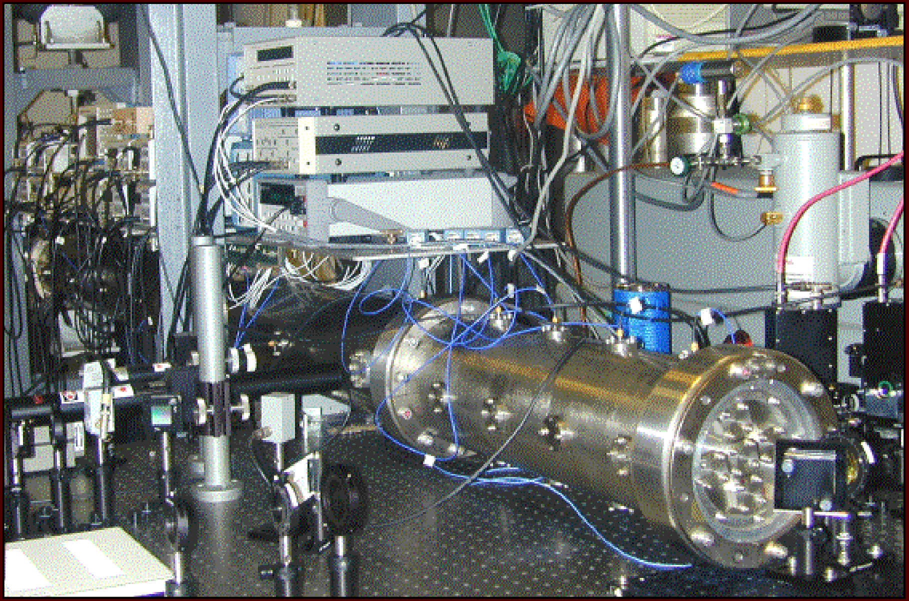
$$\mathbf{NNH + O \rightarrow NO + NH}$$

Task 5 – NOx Kinetics

Second High-Pressure Shock Tube Located at Aerospace Corp.

Aerospace High Pressure Shock-Tube Facility

- 1 – 100 atm Capability
- 600 – 4000 K Test Temperature
- 3 ms Test Time
- 3.5 m Driver and 10.7 m Driven Sections
- 16.2 cm Driven Inner Diameter



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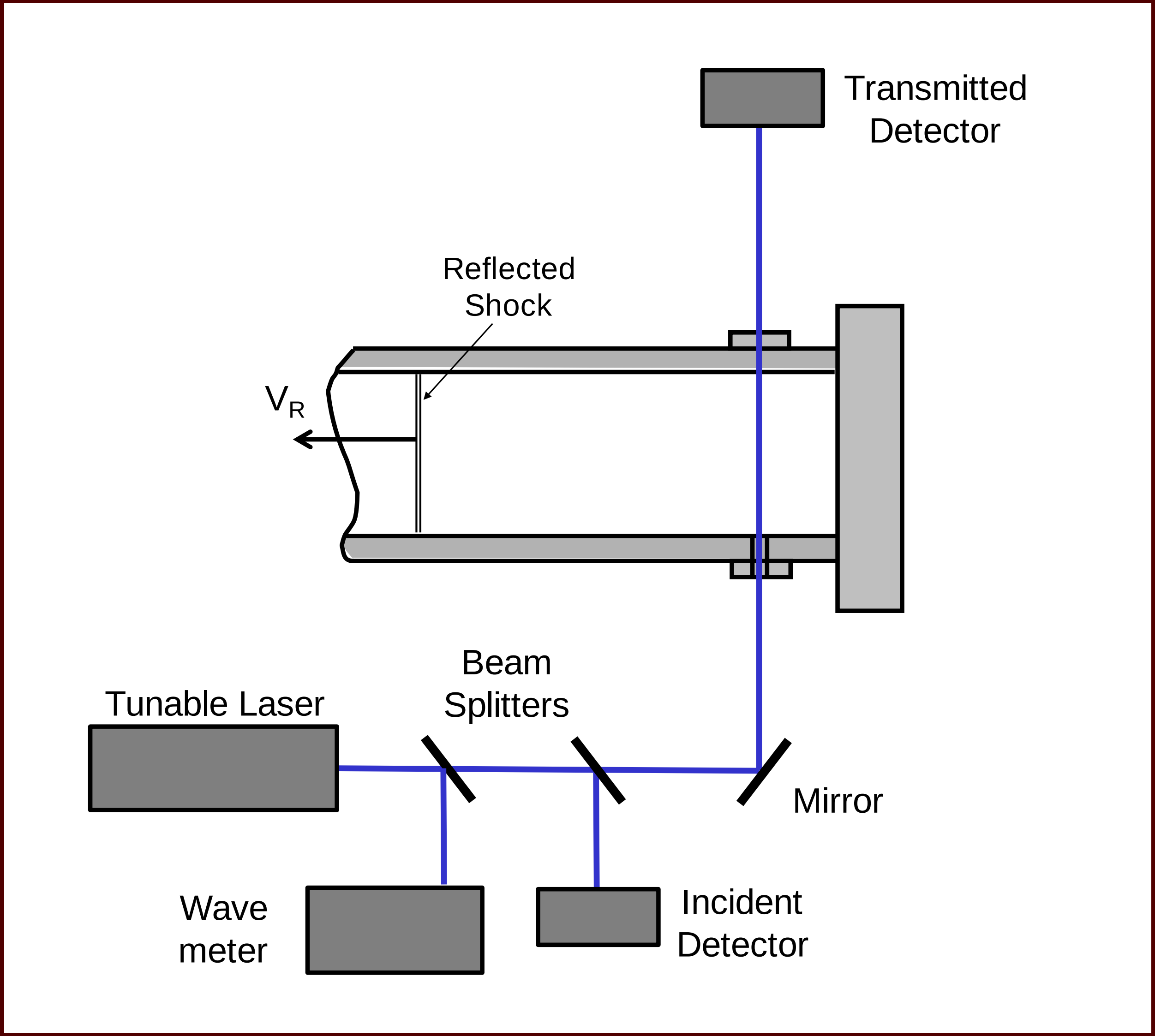
Task 5 – NOx Kinetics

Laser Absorption of NH at 336 nm Will be Targeted



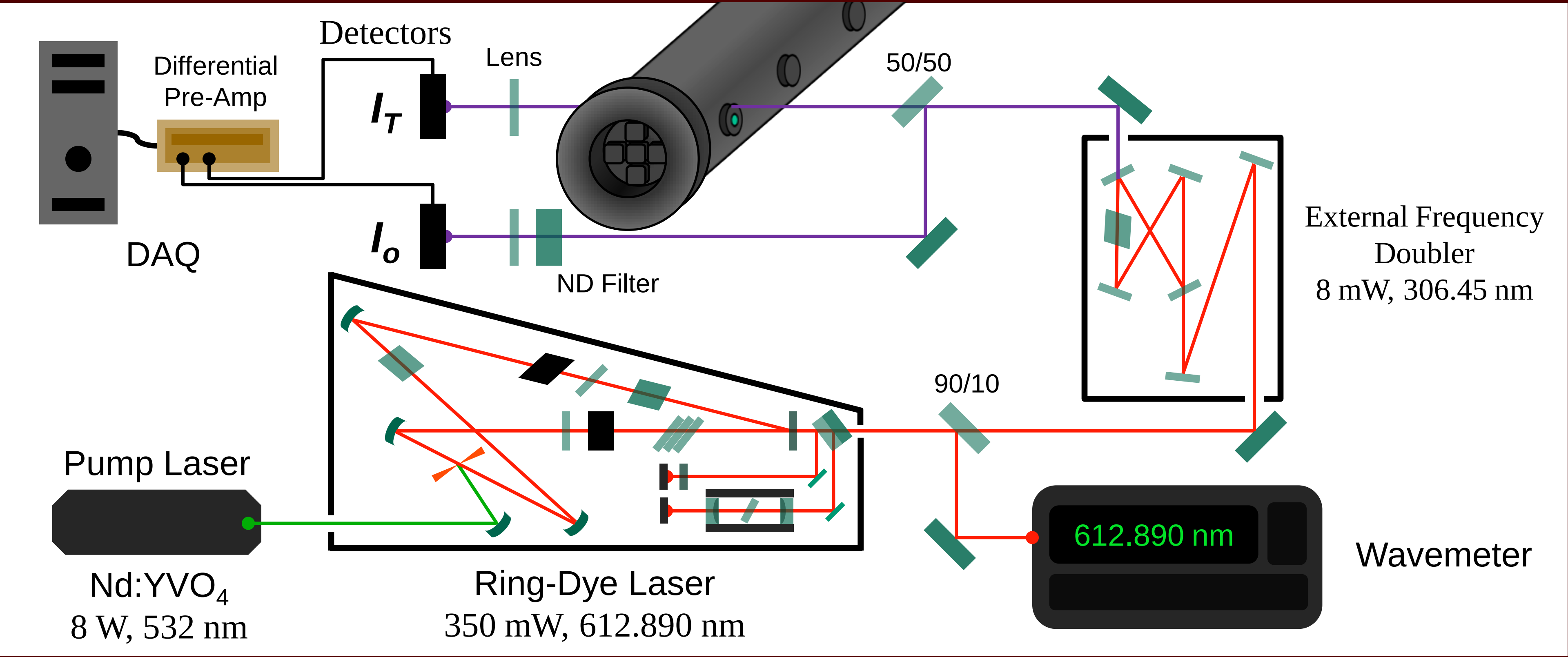
Task 5 – NOx Kinetics

Work to Date Includes Setting up and Demonstrating Laser Absorption Diagnostic

- Ring-Dye Laser System in UV
- Target OH at 307 nm to Demonstrate Diagnostic
- Future Experiments to Move to NH (336 nm)
- Kinetic and Spectroscopic Calculations for NH Underway

Task 5 – NOx Kinetics

Tunable Laser Absorption Setup



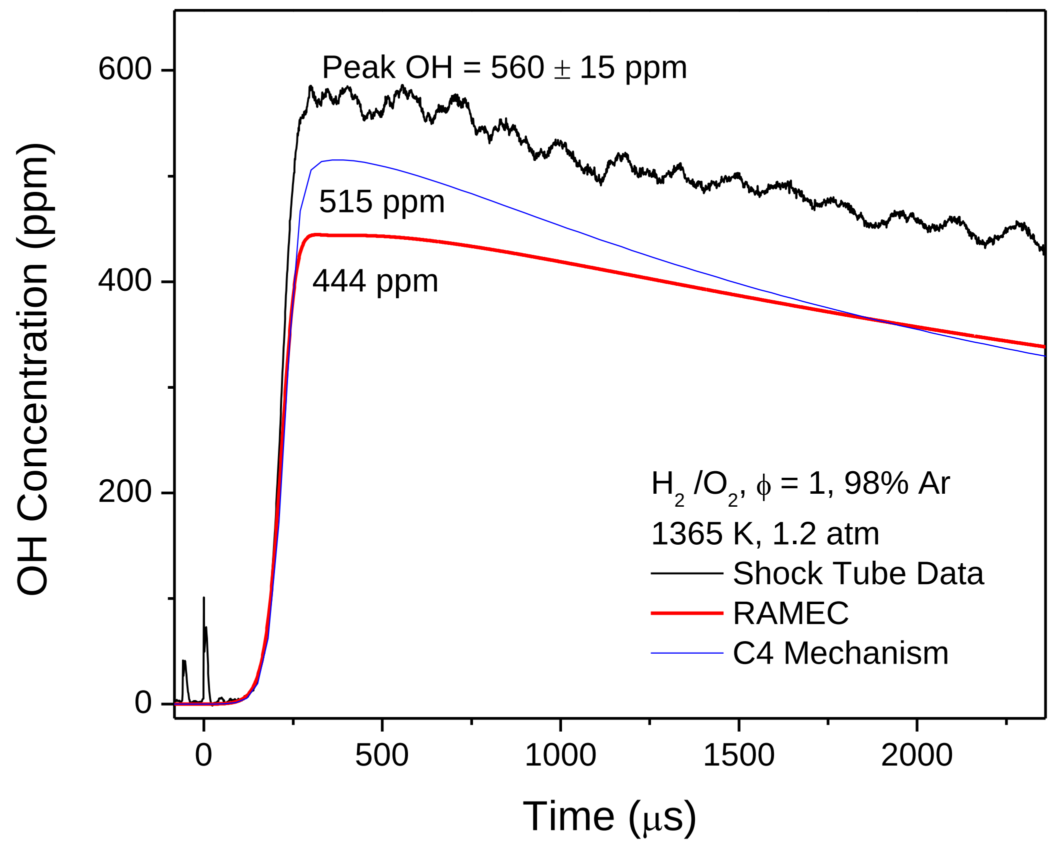
$$\frac{I_T}{I_o} = e^{-k_\nu P X_{abs} L}$$

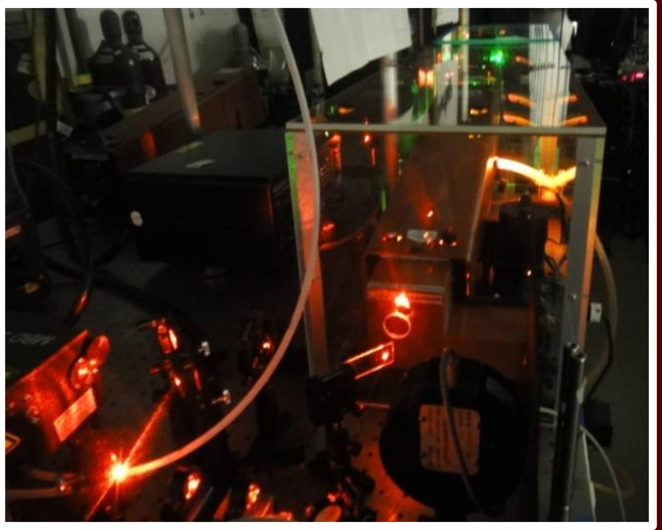
Beer-Lambert Law

- Species concentration can be found if absorption coefficient k_n is known

Task 5 – NOx Kinetics

OH Times Histories Have Been Measured in the Shock Tube





Task 6 – Effect of Impurities on Syngas Kinetics

Task 6 – Impurities

Trace Impurities Will be Studied Using Shock Tubes and Flame Speeds

- Trace Species (H_2S, NH_3, HCN, NOx, HC fuel, other?)
- Laminar Flame Speeds Using Established Methods
- Dilute Shock-Tube Experiments (Ignition and Time Histories)
- Pertinent Mixtures of Interest to Industry

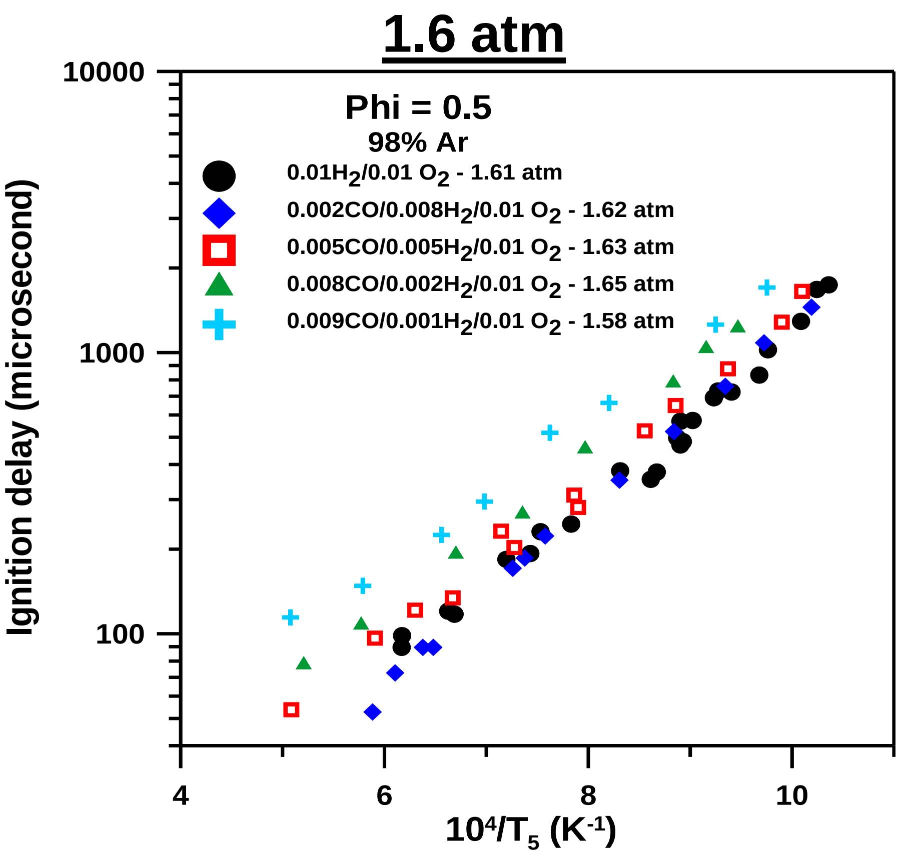
Task 6 – Impurities

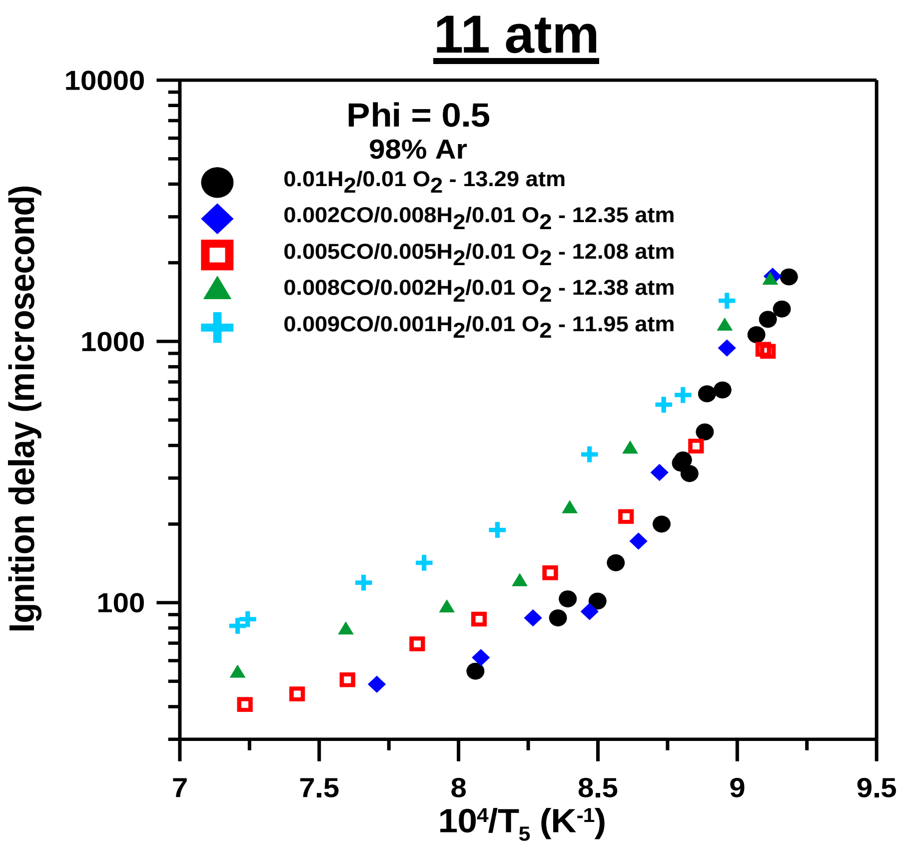
Baseline Syngas Mixtures Have Been Selected and Tested (Ignition Delay Times)

- H_2/CO Blends as Baseline:
  - H_2/CO: 80/20, 50/50, 40/60, 20/80, 10/90
  - Pressures: 1, 10, 30 atm
  - $\phi = 0.5$, high Argon Dilution (98%)
- Ignition Delay Times Obtained
- Target Syngas Baseline Blends:
  - Coal Blend (50:50 base + impurities)
  - Biomass Blend (40:60 base + impurities)

Task 6 – Impurities

Ignition Data Already Obtained for Baseline Mixtures





Task 6 – Impurities

Ongoing Test Plan for Impurities and Diluents:

- Diluent Species: **H_2O, CO_2**

- Trace Species:

  - Biomass Syngas (**CH_4, NH_3**)

  - Coal Syngas (**H_2S, NH_3, HCN, COS**)

Summary

Progress on All 6 Tasks for 1st Year Have Been Covered

Work Tasks:

Task 1 – Project Management and Program Planning

Task 2 – Turbulent Flame Speed Measurements

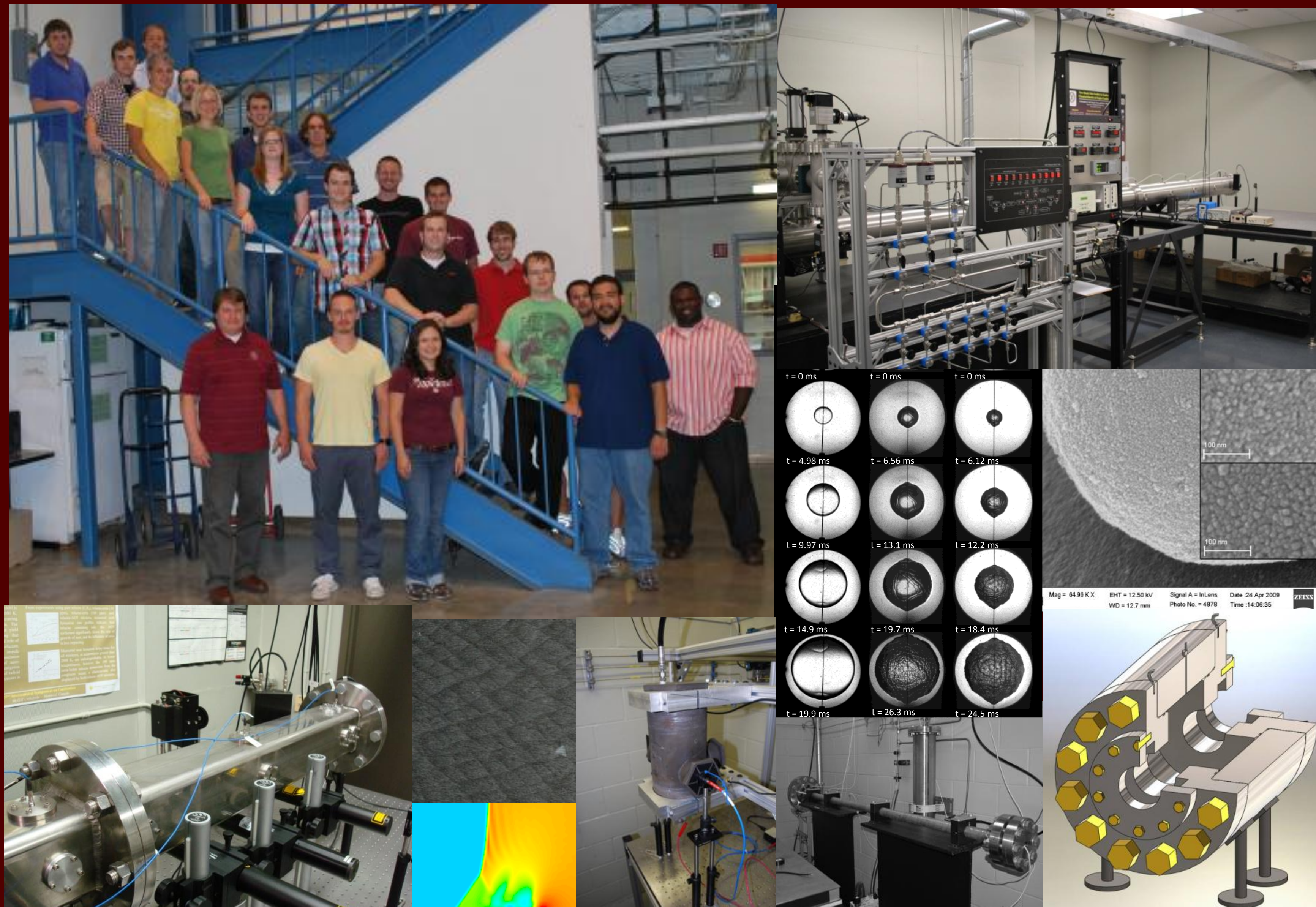
Task 3 – Laminar Flame Speeds with Diluents

Task 4 – NOx Mechanism Validation Experiments

Task 5 – Fundamental NOx Kinetics

Task 6 – Effect of Impurities on Syngas Kinetics

Petersen Group Research



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